This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

L29 0 L28

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.31	861.15

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-12.49

FILE 'REGISTRY' ENTERED AT 14:26:37 ON 13 MAR 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

STRUCTURE FILE UPDATES: 12 MAR 2001 HIGHEST RN 326849-80-3
DICTIONARY FILE UPDATES: 12 MAR 2001 HIGHEST RN 326849-80-3

TSCA INFORMATION NOW CURRENT THROUGH July 8, 2000

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT for details.

37534

U.S. DEPARTMENT OF COMMERCE
Patent and Trademark Office

SEARCH REQUEST FORM

Requestor's Name: BERCH

Serial Number: 09/554077

Date: 3/13/01

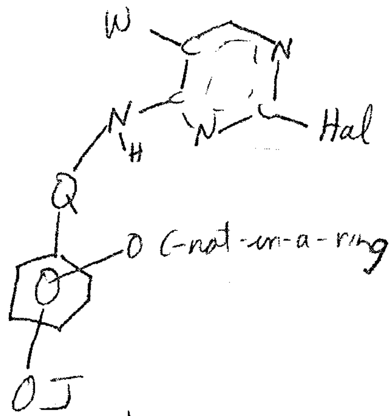
Phone: 4718 (4E12 mb)

Art Unit: 1624 (4D15)

Search Topic:

Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevent citations, authors, keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevent claim(s).

W = NH_2 or NO_2



J = C, but not —⟨phenyl⟩ (alc)

Q = $(CH_2)_{1-3}$ or —C(CH$_3$)(H)—

MARY

Point of Contact:
Mary Hale
Technical Info. Specialist
CM1 12D16 Tel: 308-4258

#2 of 2

STAFF USE ONLY

Date completed: 3/13	**Search Site**	**Vendors**
Searcher: Clary	___ STIC	___ IG
Terminal time: 30	___ CM-1	MR ___ STN
Elapsed time: 3	___ Pre-S	___ Dialog
CPU time:	**Type of Search**	___ APS
Total time:	___ N.A. Sequence	___ Geninfo
Number of Searches:	___ A.A. Sequence	___ SDC
Number of Databases:	1 Structure	___ DARC/Questel
	___ Bibliographic	___ Other

PTO-1590 (9-90)

BERCH
554077

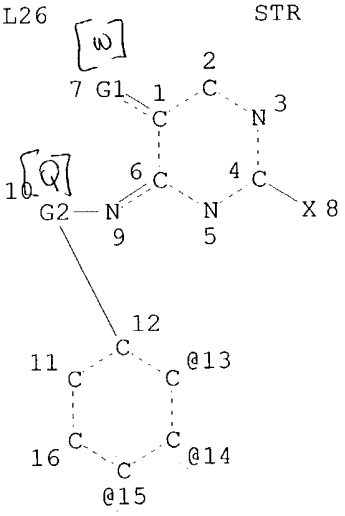
TSCA INFORMATION NOW CURRENT THROUGH July 8, 2000

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT for details.

=> d l28 que stat;d 1-4 ide cbib abs

L26 STR



ω= VAR G1=NH2/NO2
Q= REP G2=(1-3) C — open will retrieve $(CH_2)_{1-3}$ or CH_3 / CH
VPA 17-13/14/15 U
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 17

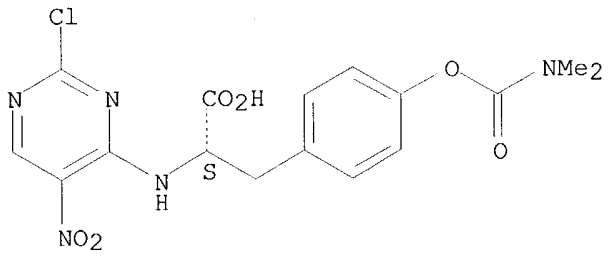
STEREO ATTRIBUTES: NONE
L28 4 SEA FILE=REGISTRY SSS FUL L26

100.0% PROCESSED 57 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.04

L28 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2001 ACS
RN 285140-23-0 REGISTRY
CN L-Tyrosine, N-(2-chloro-5-nitro-4-pyrimidinyl)-, dimethylcarbamate (ester)
(9CI) (CA INDEX NAME)

FS STEREOSEARCH
MF C16 H16 Cl N5 O6
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

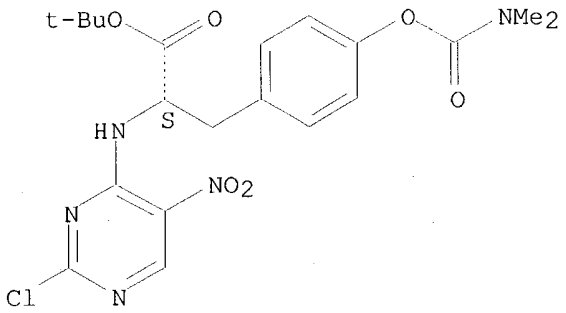
REFERENCE 1: 133:120681 Preparation of amino acid acyl derivatives as inhibitors of leukocyte adhesion mediated by VLA-4. Konradi, Andrei; Pleiss, Michael A.; Thorsett, Eugene D.; Ashwell, Susan; Welmaker, Gregory S.; Kreft, Anthony; Sarantakis, Dimitrios; Dressen, Darren B.; Grant, Francine S.; Semko, Christopher; Xu, Ying-Zi (Elan Pharmaceuticals, Inc., USA; American Home Products). PCT Int. Appl. WO 2000043372 A1 20000727, 342 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US1686 20000121.
PRIORITY: US 1999-PV116923 19990122; US 1999-PV160999 19991021.

AB Disclosed are compds. R2-W:CR1-Q-CR3R3'COX and R2-W'-CHR1-Q-CR3R3'COX [R1 and R2 are joined to form a ring; R3, R3' = H, iso-Pr, -CH2Z or :CHZ, where Z = H, acylamino, alkyl, alkoxy, aryloxy, aryl, aryloxyaryl, carboxy, carboxyalkyl, etc.; Q = O, S, SO, SO2, NH or imino group; W = nitrogen, carbon; W' = nitrogen, carbon, oxygen, sulfur, SO, SO2; X = OH, (un)substituted alkoxy, alkenoxy, cycloalkoxy, cycloalkenoxy, aryloxy, heteroaryloxy or heterocyclyloxy, an amino group] which bind VLA-4. Thus, N-[5-(N-4-toluenesulfonylamino)pyrimidin-4-yl]-L-4-(N,N-dimethylcarbamyloxy)phenylalanine tert-Bu ester was prepd. by condensation of L-4-(N,N-dimethylcarbamyloxy)phenylalanine tert-Bu ester with 2,4-dichloro-5-nitropyrimidine, followed by nitro group redn. and tosylation. Compds. synthesized in the examples are expected to have a binding affinity to VLA-4 expressed by an IC50 of 15 .mu.M or less.

L28 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2001 ACS
RN 285139-31-3 REGISTRY

CN L-Tyrosine, N-(2-chloro-5-nitro-4-pyrimidinyl)-, 1,1-dimethylethyl ester, dimethylcarbamate (ester) (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H24 Cl N5 O6
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



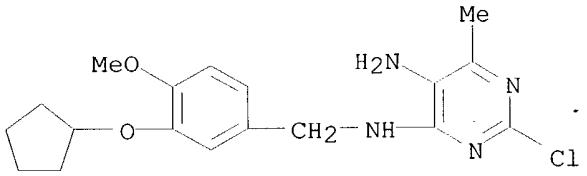
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:120681 Preparation of amino acid acyl derivatives as inhibitors of leukocyte adhesion mediated by VLA-4. Konradi, Andrei; Pleiss, Michael A.; Thorsett, Eugene D.; Ashwell, Susan; Welmaker, Gregory S.; Kreft, Anthony; Sarantakis, Dimitrios; Dressen, Darren B.; Grant, Francine S.; Semko, Christopher; Xu, Ying-Zi (Elan Pharmaceuticals, Inc., USA; American Home Products). PCT Int. Appl. WO 2000043372 A1 20000727, 342 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US1686 20000121.
PRIORITY: US 1999-PV116923 19990122; US 1999-PV160999 19991021.

AB Disclosed are compds. R2-W:CR1-Q-CR3R3'COX and R2-W'-CHR1-Q-CR3R3'COX [R1 and R2 are joined to form a ring; R3, R3' = H, iso-Pr, -CH2Z or :CHZ, where Z = H, acylamino, alkyl, alkoxy, aryloxy, aryl, aryloxyaryl, carboxy, carboxyalkyl, etc.; Q = O, S, SO, SO2, NH or imino group; W = nitrogen, carbon; W' = nitrogen, carbon, oxygen, sulfur, SO, SO2; X = OH, (un)substituted alkoxy, alkenoxy, cycloalkoxy, cycloalkenoxy, aryloxy, heteroaryloxy or heterocyclyloxy, an amino group] which bind VLA-4. Thus, N-[5-(N-4-toluenesulfonylamino)pyrimidin-4-yl]-L-4-(N,N-dimethylcarbamyloxy)phenylalanine tert-Bu ester was prepd. by condensation of L-4-(N,N-dimethylcarbamyloxy)phenylalanine tert-Bu ester with 2,4-dichloro-5-nitropyrimidine, followed by nitro group redn. and tosylation. Compds. synthesized in the examples are expected to have a

binding affinity to VLA-4 expressed by an IC50 of 15 .mu.M or less.

L28 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2001 ACS
RN 225100-33-4 REGISTRY
CN 4,5-Pyrimidinediamine, 2-chloro-N4-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-6-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H23 Cl N4 O2
SR CA
LC STN Files: CA, CAPLUS



2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

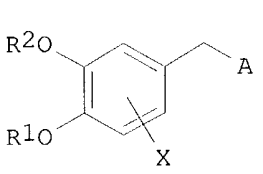
REFERENCE 1: 133:350245 Preparation of purine derivative dihydrate as phosphodiesterase IV inhibitor. Sekiya, Kouichi; Takemiya, Akihiro; Ohshima, Masahiro (Mitsubishi Chemical Corporation, Japan). PCT Int. Appl. WO 2000068231 A1 20001116, 29 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (Japanese). CODEN: PIXXD2. APPLICATION: WO 2000-JP2952 20000509. PRIORITY: JP 1999-129499 19990511.

AB Claimed is a dihydrate of 4-[[9-[(3-cyclopentyloxy-4-methoxy)benzyl]-6,8-dimethylpurin]-2-yl-3-oxypropyl]pyridine N-oxide (I); also claimed are : (a) pharmaceutical contg. I as active ingredient; (b) pharmaceutical contg. I as active ingredient for the treatment of asthma, chronic obstructive lung disease and/or other inflammatory diseases; (c) phosphodiesterase IV inhibitor contg. I (d) and intermediates for I. I in vitro showed IC50 of 3.4 x 10-9 M against phosphodiesterase IV, vs. IC50 of 5 x 10-7 M shown by rolipram.

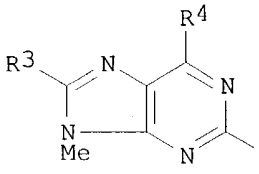
REFERENCE 2: 130:352279 Preparation of purine derivatives as antiasthmatics. This one

Tanaka, Toshihiko; Iwashita, Eiichirou; Tarao, Akiko; Amenomori, Akira; Ono, Yuya (Mitsubishi Chemical Corporation, Japan). PCT Int. Appl. WO 9924432 A1 19990520, 148 pp. DESIGNATED STATES: W: CA, CN, GB, KR, US; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (Japanese). CODEN: PIXXD2. APPLICATION: WO 1998-JP5092 19981112. PRIORITY: JP 1997-310365 19971112.

GI



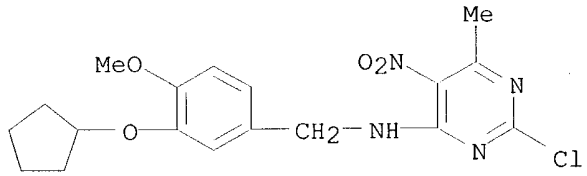
I



II

AB Title compds. I and II (R1 = alkyl, CHF2; R2 = tetrahydrofuranyl, alkyl, haloalkyl, alkenyl, cycloalkyl, etc.; R3 = H, halo, OH, alkyl, alkoxy, amino, alkylamino, dialkylamino, etc; R4, R5 = H, halo, alkyl, alkoxy, amino, alkylamino, pyrrolidinyl, morpholino, dialkylamino, etc; X = H, halo, NO2) and their salts, useful as antiasthmatics, were prepd. 2-Chloro-9-[(3-cyclopentyloxy-4-methoxy)benzyl]-6,8-dimethylpurine showed IC50 of 6.7 x 10-9 M against phosphodiesterase IV. Formulations contg. title compds. were given.

L28 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2001 ACS
RN 225100-31-2 REGISTRY
CN 4-Pyrimidinamine,
2-chloro-N-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-
6-methyl-5-nitro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H21 Cl N4 O4
SR CA
LC STN Files: CA, CAPLUS



2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:350245 Preparation of purine derivative dihydrate as phosphodiesterase IV inhibitor. Sekiya, Kouichi; Takemiya, Akihiro; Ohshima, Masahiro (Mitsubishi Chemical Corporation, Japan). PCT Int. Appl. WO 2000068231 A1 20001116, 29 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (Japanese). CODEN: PIXXD2. APPLICATION: WO 2000-JP2952 20000509. PRIORITY: JP 1999-129499 19990511.

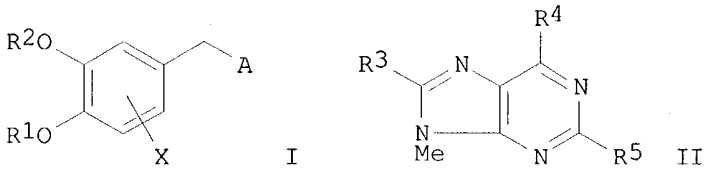
AB Claimed is a dihydrate of 4-[[9-[(3-cyclopentyloxy-4-methoxy)benzyl]-6,8-dimethylpurin]-2-yl-3-oxypropyl]pyridine N-oxide (I); also claimed are ;

(a) pharmaceutical contg. I as active ingredient; (b) pharmaceutical contg. I as active ingredient for the treatment of asthma, chronic obstructive lung disease and/or other inflammatory diseases; (c) phosphodiesterase IV inhibitor contg. I (d) and intermediates for I. I in vitro showed IC50 of 3.4 x 10-9 M against phosphodiesterase IV, vs. IC50 of 5 x 10-7 M shown by rolipram.

REFERENCE 2: 130:352279 Preparation of purine derivatives as antiasthmatics.

Tanaka, Toshihiko; Iwashita, Eiichirou; Tarao, Akiko; Amenomori, Akira; Ono, Yuya (Mitsubishi Chemical Corporation, Japan). PCT Int. Appl. WO 9924432 A1 19990520, 148 pp. DESIGNATED STATES: W: CA, CN, GB, KR, US; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (Japanese). CODEN: PIXXD2. APPLICATION: WO 1998-JP5092 19981112. PRIORITY: JP 1997-310365 19971112.

GI



AB Title compds. I and II (R1 = alkyl, CHF2; R2 = tetrahydrofuranyl, alkyl, haloalkyl, alkenyl, cycloalkyl, etc.; R3 = H, halo, OH, alkyl, alkoxy, amino, alkylamino, dialkylamino, etc; R4, R5 = H, halo, alkyl, alkoxy, amino, alkylamino, pyrrolidinyl, morpholino, dialkylamino, etc; X = H, halo, NO2) and their salts, useful as antiasthmatics, were prepd. 2-Chloro-9-[(3-cyclopentyloxy-4-methoxy)benzyl]-6,8-dimethylpurine showed IC50 of 6.7 x 10-9 M against phosphodiesterase IV. Formulations contg. title compds. were given.

=> fil caold;s l28

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	149.08	860.84

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.24	-12.49

FILE 'CAOLD' ENTERED AT 14:26:32 ON 13 MAR 2001

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)